

8-Azabicyclo[3.2.1]octane, 3-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)oxy]tropane

Other names:
endo-

Deptropine

3-[10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-yloxy]tropane

Dibenzheptropine

endo-3-[(10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)oxy]-8-methyl-8-azabicyclo[3.2.1]octane

Inchi: InChI=1S/C23H27NO/c1-24-18-12-13-19(24)15-20(14-18)25-23-21-8-4-2-6-16(21)10-11

InchiKey: ZWPODSUQWXAZNC-UHFFFAOYSA-N

Formula: C23H27NO

SMILES: CN1C2CCC1CC(OC1c3ccccc3CCc3ccccc31)C2

Mol. weight [g/mol]: 333.47

CAS: 604-51-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.83		Crippen Method
logp	4.516		Crippen Method
mcvol	270.680	ml/mol	McGowan Method
rinpol	2650.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2650.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C604513&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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